Validation Test Report for the Variational Assimilation of Satellite Sea Surface Temperature Radiances

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14. ABSTRACT

Validation of an observation operator developed for direct assimilation of satellite sea surface temperature (SST) radiances using radiative transfer modeling is provided. The radiance assimilation operator has been integrated into the Navy Coupled Ocean Data Assimilation ocean data quality control and three dimensional variational analysis (3DVAR) systems. The operator uses an incremental approach. It takes as input prior estimates of SST from an ocean forecast model and profiles of atmospheric state variables (specific humidity, air temperature) known to affect satellite SST radiances. Observed radiances are simulated usng a fast radiative transfer model. Differences between observed and simulated radiances are used to force a SST inverse model. The inverse model outputs the change in SST that takes into account the variable temperature and water vapor content of the atmosphere at the time and location of the satellite radiance measurement. These SST corrections are then assimilated with other ocean observations in the 3DVAR.

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Executive Summary

Validation and description of an observation operator developed for direct assimilation of satellite SST radiances using radiative transfer modeling is provided. The radiance assimilation operator has been integrated into the Navy Coupled Ocean Data Assimilation ocean data quality control and three dimensional variational analysis systems. The operator uses an incremental approach. It takes as input prior estimates of SST from an ocean forecast model and profiles of atmospheric state variables known to affect satellite SST radiances. Currently these variables include specific humidity and air temperature, which are routinely available from Navy numerical weather prediction systems. Observed radiances are simulated using a fast radiative transfer model. Differences between observed and simulated radiances are used to force a SST inverse model. The inverse model outputs the change in SST that takes into account the variable temperature and water vapor content of the atmosphere at the time and location of the satellite radiance measurement. These SST corrections are treated as innovations in the variational minimization, and assimilated simultaneously with other observations of ocean temperature, salinity, and velocity. Direct assimilation of satellite SST radiances is a true example of coupled data assimilation. An observation in one fluid (atmospheric radiances) creates an innovation in a different fluid (ocean surface temperature). The radiance assimilation operator is ideally suited for coupled ocean/atmosphere forecasting systems where the atmosphere and ocean states have evolved consistently over time.

1.   Introduction

Accurate representation of the sea surface temperature (SST) is critical to both meteorology and oceanography. Operational uses of SST include numerical weather prediction (NWP) where the SST information is used to prescribe the lower temperature boundary condition over the ocean, and short-range ocean forecasting in which SST data are assimilated during initialization. Global SST has been observed routinely by satellites since the early 1980s. Satellite radiometers measure top-of-the-atmosphere brightness temperatures (TOA-BTs), or radiances, in the relevant regions of the infrared spectrum (3.4 to 4.1 µm and 10.5 to 12 µm). Retrievals of SST from these space-based measurements are typically empirically determined by regression of radiance observations matched to *in situ* SST (McClain *et al.*, 1985). More recently, however, satellite SST retrievals are increasingly based on results of radiative transfer simulations (Merchant et al., 2008). The purpose of this report is to provide a description and validation of an observation operator for direct assimilation of satellite SST radiances using radiative transfer modeling. The operator was developed in the *"Variational Assimilation of Satellite Sea Surface Temperature Radiances"* project.   The project was supported by PMW-120 under Program Element 0603207N.

The validation test report is organized as follows: section 2 gives an overview of sea surface temperature measurements and radiative transfer modeling; section 3 describes the SST radiance assimilation operator; section 4 outlines application of the operator in the Navy Coupled Ocean Data Assimilation (NCODA) analysis and quality control systems; and section 5 provides the validation test results. Operational implementation of the SST radiance assimilation capability at the Navy operational centers is described in section 6, and future development possibilities are summarized in section 7.

Transition of the SST radiance assimilation capability from development within the Naval Research Laboratory (NRL) to operational evaluation at Fleet Numerical Meteorology and Oceanography Center (FNMOC) and Naval Oceanographic Office (NAVOCEANO) is being done in accordance with the Memorandum of Understanding between NRL, NAVOCEANO, and

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FNMOC, detailed in COMNAVOCEANCOM ltr 3140 ser 5/076 of 14 Feb 1990. The SST radiance assimilation Transition Validation Panel (TVP) is comprised of the following individuals: James Cummings (NRL-SSC, Chair), James Peak (NRL-MRY), Mark Ignaszewski (FNMOC), Keith Willis (NAVOCEANO), and Piotr Flatau (Scripps Institution of Oceanography), who served as the outside expert. The members of the TVP assisted in the drafting of the model transition plan and have reviewed the outcomes of the test plan documented in this validation test report.

2.   SST Measurements and Radiative Transfer Modeling

Remotely sensed SST is estimated from TOA-BTs seen by broad thermal channels located in window regions of the atmospheric transmittance spectrum. These channels are nominally centered on wavelengths of 3.7 μm, 11 μm, and 12 μm. Of these the 3.7 μm channel is used for estimation of SST only at night because of the possibility of contamination by reflected solar irradiance during the day. Thus, different combinations of channels are used during day and night to estimate SST. Radiances observed by satellite-based infrared sensors can only be used as the sensor views the ocean under clear-sky conditions. In the discussion that follows it is assumed that this important cloud-screening step has been adequately achieved.

The TOA-BT in the atmospheric window portion of the infrared spectrum is largely determined by the ocean surface temperature, the total-column water-vapor (TCWV) present in the atmosphere, the broad vertical distribution of the atmospheric water vapor, and the near-surface vertical distribution of atmospheric temperature. These features of the ocean surface and atmospheric state vary on a range of scales. TCWV over the oceans is a maximum in the equatorial zone and reduces towards high latitudes. Atmospheric temperatures similarly decrease with increasing latitude. Within latitude zones, large-scale circulations affect both the total-column and vertical distribution of water vapor, and there is considerable variability associated with the presence of land masses. Air–sea temperature difference can vary on relatively short spatial scales as SST changes more rapidly than the temperature of the lower atmosphere in upwelling areas and across ocean fronts. This variability is reflected to varying degree in the observed TOA-BTs, which can be expected to have similar temporal and geographical variations.

Assimilation of satellite radiances requires a fast and accurate radiative transfer model (RTM) to simulate the observed radiances. This simulation is referred to as the forward model and has several elements. One element, of course, is the actual RTM software. For this purpose we use the Community Radiative Transfer Model (CRTM), shared software developed and maintained by the Joint Center for Satellite Data Assimilation (JCSDA) for national operational use by NOAA, NASA, Air Force, and Navy. The second element of the RTM is the spectral response function that characterizes the sensor. RTM calculations are based on spectroscopic parameters for various atmospheric gases and aerosols. The spectroscopic parameters embody measurements of the many weak absorption features in the relevant regions of the infrared spectrum. These parameters and other sensor characterizations are contained in satellite specific coefficient data bases that are loaded when CRTM is initialized for a specific satellite and instrument package. The third element of the forward model is a set of atmospheric profiles and associated surface variables (SST) that are representative of the atmospheric state through which the sensor has observed surface emissions of infrared energy.

Radiance assimilation inversion techniques require the accompanying Jacobian for the forward model. The Jacobian is the partial derivative of the radiance with respect to the atmospheric and ocean surface parameters influencing that radiance. The Jacobian is fundamental in radiance assimilation as its magnitude and shape determine the magnitude and shape of the corrections to a first guess. The Jacobian is obtained by perturbation of the inputs to the forward model, but this approach is extremely costly to compute. Here, we take advantage of CRTM software that performs the forward modeling and returns the Jacobian tangent linear outputs for all of the prior information used to simulate the radiances in a single subroutine call.

3. Radiance Assimilation Observation Operator

The radiance assimilation observation operator has been incorporated into the NCODA ocean data quality control (NCODA QC), and the NCODA three-dimensional variational analysis (NCODA 3DVAR) systems. The operator uses an incremental approach. It takes as input prior estimates of SST along with profiles of atmospheric state variables known to affect satellite SST radiances. Currently, the variables considered in the operator include specific humidity, air

temperature, and SST. All of these variables are routinely available from Navy NWP and ocean forecasting systems. The operator is forced by differences between observed and predicted TOA-BTs for the different satellite SST instrument channel wavelengths. Output of the operator is the change in SST that takes into account the variable temperature and water vapor content of the atmosphere at the time and location of the satellite radiance measurement. When cycling in the NCODA 3DVAR sequential incremental update cycle these SST corrections are treated as innovations and assimilated with other observations of ocean temperature, salinity, and velocity in the minimization.

Figure 1 presents a schematic of the satellite SST radiance assimilation operator. The upper left hand side of the figure shows input of the satellite radiance observations. Prior to use in the operator the satellite radiance data must be calibrated, geo-located, quality controlled, and cloud
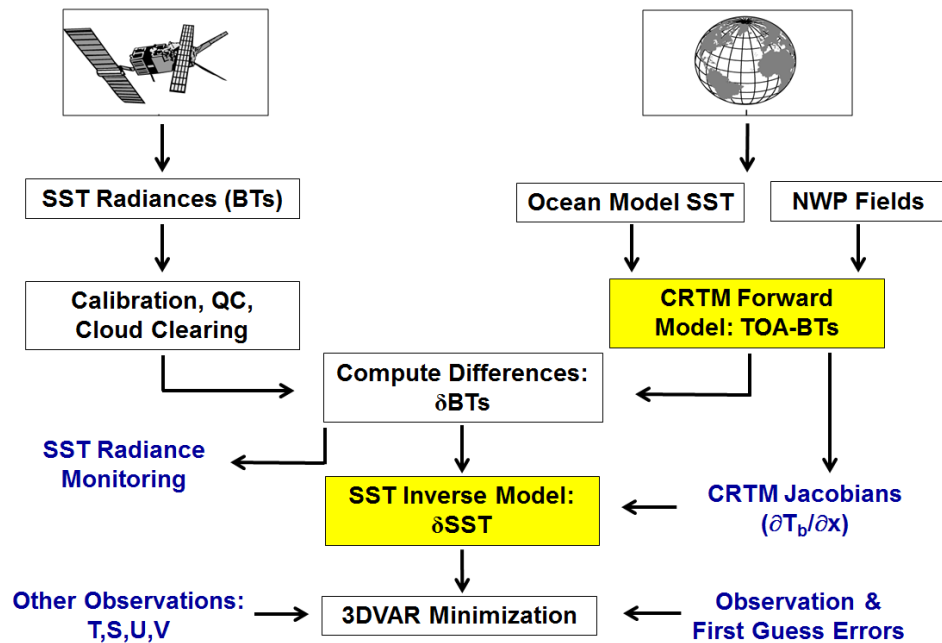
Figure 1. Schematic of the process for direct assimilation of satellite SST radiances using radiative transfer modeling.   See text for details on the highlighted CRTM forward modeling and SST inverse modeling components of the operator.

cleared. This processing is performed by NAVOCEANO. NAVOCEANO also does averaging of several fields of view in a 2x2 target where all pixels in the target must be cloud free. The field of view averaging smooth out pixel-level differences and has been shown to return a more accurate SST (May and Osterman, 1998). As a result of the extensive quality control and field of

view averaging, the NAVOCEANO radiance data are of high quality and generally do not require further quality control. However, as will be shown, the atmospheric correction computed as part of the SST inverse model provides additional information that can be used to screen the data and reject what otherwise are undetected outliers. In addition to the satellite radiance data, the radiance assimilation operator needs the satellite geometry information. This includes the sensor zenith, solar zenith, and solar azimuth angles. Currently, satellite radiance observations available from NAVOCEANO include: GOES-13, GOES-15, NOAA-18, NOAA-19, METOP-A, METOP-B, and NPP-VIIRS. The operator is also set up to process SST radiance data from COMS-1, the Korean geostationary satellite, but NAVOCEANO funding for receiving and processing COMS-1 data was cut. These data will automatically be processed by the operator once funding is restored and the flow of COMS-1 data resumes. It should also be noted that NAVOCEANO does not process all sources of satellite SST radiances. Radiance measurements from the geostationary MSG and MTSAT-2 satellites are not available at this point in time. These satellites are defined in the CRTM coefficient data base and can be added to the radiance assimilation operator once clear-sky TOA-BTs are available.

The upper right hand side of Figure 1 shows input of the prior estimates of the SST and atmospheric state variables. The Navy Global Environmental Model (NAVGEM) is used to provide three-dimensional fields of specific humidity and air temperature. NAVGEM is executed on a T359 Gaussian grid (~33 km resolution) with 50 sigma levels. The model fields are available at 3-hourly forecast periods on a 0.5 degree spherical application grid (~55 km) with 26 pressure levels. NAVGEM fields are not interpolated to the locations of the satellite SST radiance observations. Rather, collocations are done on the basis of nearest neighbor. In that regard, the atmospheric state is known within a time range of not more than 90 minutes and a spatial radius of less than 27 km for the observed TOA-BTs. The prior SST is obtained from the Navy's Global Ocean Forecast System (GOFS), which is based on the HYbrid Coordinate Ocean Model (HYCOM). HYCOM is executed on a global 1/12 degree resolution grid and is forced by NAVGEM. The prior SST for the radiance assimilation operator is interpolated from hourly HYCOM forecast fields to the TOA-BT observation location using the first guess at appropriate time (FGAT) method.

The CRTM forward model generates simulated radiances at the observation locations given the satellite channel wavelength and ocean and atmosphere prior information. Differences between radiances observed by the satellite and those obtained from the forward model simulations are formed. These differences are used to force the SST inverse model. The SST inverse model partitions the radiance differences into physical corrections for atmospheric temperature, water vapor, and SST. The SST inverse model for a given channel is given by,

$$
\begin{bmatrix} \delta BT \cdot J_{sst} \\ \delta BT \cdot J_{t} \\ \delta BT \cdot J_{q} \end{bmatrix} = \begin{bmatrix} \varepsilon_{sst}^{-1} \cdot J_{sst} \cdot J_{sst} & J_{sst} \cdot J_{t} & J_{sst} \cdot J_{q} \\ J_{t} \cdot J_{sst} & \varepsilon_{t}^{-1} \cdot J_{t} \cdot J_{t} & J_{t} \cdot J_{q} \\ J_{q} \cdot J_{sst} & J_{q} \cdot J_{t} & \varepsilon_{q}^{-1} \cdot J_{q} \cdot J_{q} \end{bmatrix} \begin{bmatrix} \delta T_{sst} \\ \delta T_{a} \\ \delta Q_{a} \end{bmatrix}
\tag{1}
$$

where δBT is the TOA-BT difference (or innovation), J_{sst}, J_{t}, and J_{q} are the radiative transfer model Jacobians, and ε_{sst}, ε_{t}, and ε_{q} are the prior errors for SST, atmospheric temperature, and water vapor, respectively. The SST inverse model is solved analytically for the δT_{sst}, δT_{a}, and δQ_{a} prior corrections. The corrections are calculated independently and summed over each of the SST channels (3 channels at night, 2 channels during the day) to obtain the total prior corrections. SST corrections calculated in this way take into account the variable temperature and water vapor content of the atmosphere at the time and location of the radiance measurement. With this approach, coefficients that relate radiances to SST in the observation operator are dynamically defined for each atmospheric situation observed. The method removes atmospheric signals in the radiance data and in the process extracts more information on the SST. A similar SST inverse model is in use at NCEP for producing *physical* SST retrievals from satellite SST radiances (Derber *et al.*, 2003).

The SST inverse model requires careful consideration of the biases and error statistics of the NWP and SST priors. Biases are expected since the NWP information may represent areas that are both cloudy and clear, while the satellite SST radiance measurements, by definition, are only available in clear-sky, cloud free conditions. These discrepancies may be due to atmospheric model error or more likely simply due to resolution differences between the NAVGEM model fields (~55 km) and the high resolution infrared satellite SST data (~1 km). Accordingly, a bias correction of the NAVGEM fields has been developed (see section 5). Proper specification of the error statistics of the priors in Eq. 1 is also required to correctly partition the observed TOA-

BT differences into the various sources of variability (atmospheric temperature, water vapor, or SST). The 80 member NAVGEM ensemble operational at FNMOC is used to specify variability of the deterministic atmospheric model temperature and specific humidity fields. The surface temperature background error standard deviations from the NCODA 3DVAR ocean data assimilation component of GOFS are used to define the SST prior error (Cummings and Smedstad, 2013). These fields provide situation dependent prior error statistics that vary with location and evolve with time. The combined effect of radiometric noise in the satellite BTs and forward modeling errors are estimated from variability of the δBT innovations calculated at the same time as the NAVGEM bias correction. These errors are assumed to be uncorrelated between satellite channels in the SST inverse model.

4. Application

There are two applications of the satellite SST radiance assimilation operator. The CRTM forward and SST inverse modeling are the same in the two applications. The applications differ only in the source of the prior information used in the operator, primarily the prior SST and its error estimate. The two applications are described here:

Atmospheric Correction of Empirical SST. NAVOCEANO produces empirically derived SST retrievals using regression analyses between satellite SST radiances and drifting buoy SSTs. The regressions are global, calculated once, and held constant. The regression coefficients represent a very broad range of atmospheric conditions with the result that subtle systematic errors are introduced into the empirical SST when the method is uniformly applied to new radiance data. Most notably the NAVOCEANO SST retrievals show unrealistic temporal variation in the tropics due to the unaccounted for short-term variability of the atmospheric moisture fields. As has been noted, the radiance assimilation operator dynamically corrects the prior SST for atmospheric conditions at a particular time and place. By using the empirically derived NAVOCEANO SST as the prior the operator essentially provides an "atmospheric correction" that varies on synoptic time and space scales. As will be shown, the operator also corrects a systematic error in the NAVOCEANO SST retrievals that varies geographically. This application of the operator has been integrated into the NCODA QC system. The operator computes the atmospheric correction for the NAVOCEANO SST retrievals received in a real-

time QC data cut at the center. The SST corrections are saved with the NAVOCEANO SST data in the NCODA QC system output files. These pre-calculated corrections can then be applied at the time the NAVOCEANO SST data are assimilated via a namelist variable setting in the NCODA 3DVAR system.

Ocean Data Assimilation. The radiance assimilation operation has also been integrated into the NCODA 3DVAR analysis system.   Here, TOA-BTs are selected for assimilation if the observations fall within the space/time window defined for the assimilation synoptic data cut. The atmospheric model that is used to force the ocean model provides the specific humidity and air temperature priors for the operator. The CRTM forward and SST inverse models are applied as previously described. The resulting SST correction is assimilated as an innovation along with other data selected for the analysis. This application of the operator performs direct assimilation of the satellite SST radiances. There is no need for an empirical SST derived from drifting buoy matchups.   It is a true example of coupled data assimilation, which can be defined as an observation in one fluid (atmospheric radiances) creating an innovation in a different fluid (ocean surface temperature). The radiance assimilation operator is ideally suited for coupled atmosphere/ocean forecasting systems, where the atmosphere and ocean states have evolved consistently over time.

5.   Results

Forward Modeling. Figure 2 shows scatter plots of observed TOA-BTs vs. simulated BTs from the CRTM forward modeling.   The observed radiance data were obtained from the NAVOCEANO buoy matchup data base for the time period 28 August to 5 September, 2013. Prior information for the forward model came from the NAVGEM NWP model and the NAVOCEANO empirical SST retrieval. No bias correction has been applied to the NAVGEM priors. Results are plotted for the 3.7 μm, 11 μm, and 12 μm wavelengths (channels 3, 4, 5) on 3 different satellites (METOP-A, NOAA-18, NPP-VIIRS).   Day and night data are combined in the channel 4 and 5 plots.   Only nighttime data is represented in the channel 3 plots. Atmospheric transmittance is very high for the 3.7 μm channel 3 data, which is illustrated by the low scatter in the data.   The atmosphere is essentially transparent at this wavelength.   The increase in the scatter of the channel 4 and 5 simulations is due to the variable magnitude of the
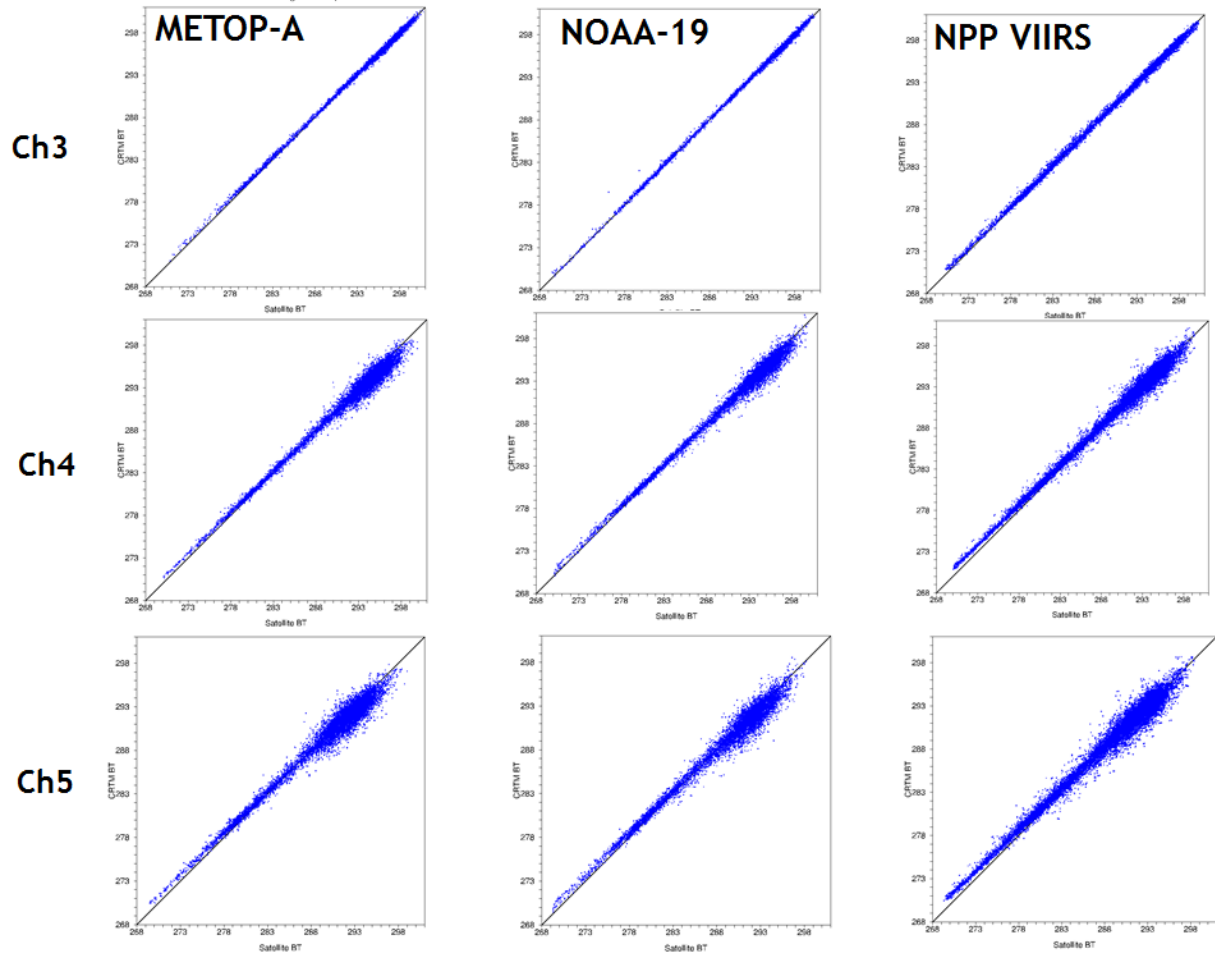
Figure 2. Scatter plots of observed (x-axis) versus radiative transfer model simulated (y-axis) brightness temperatures for METOP-A, NOAA-19, and NPP-VIIRS satellites (columns) and instrument channels (rows).

water vapor absorption. The scatter is higher at higher temperatures, which is consistent with measurements that show for moist, tropical atmospheres most of the radiation observed by satellite radiometers actually originates from the atmosphere at those wavelengths (Saunders and Edwards, 1989).

Bias Correction. The SST radiance assimilation observation operator assumes that the prior information is unbiased. In addition, the method assumes the forward model is unbiased. Any biases in these inputs to the operator will lead to corresponding biases in the output corrections. Since the NAVOCEANO SST retrievals are derived from drifting buoy matchups there is negligible bias in the SST prior. However, as mentioned previously, we expect some bias

between the NWP model outputs and the actual atmosphere observed by the satellite radiometers because the satellite radiance data are obtained from clear sky conditions while the NWP model fields may include areas that are both cloudy and clear. Following Merchant *et al*. (2008), we use an "observed" atmospheric correction to diagnose bias in the NWP fields. The observed atmospheric correction is the difference between observed and derived surface temperatures and observed and simulated radiances given by,

$$d = \left(SST_{navo} - BT_{crtm}\right) - \left(SST_{buoy} - BT_{sat}\right) \tag{2}$$

where SST_{navo} is the NAVOCEANO empirical SST retrieval, BT_{crtm} is the forward model simulated TOA-BT, SST_{buoy} is the drifting buoy SST, and BT_{sat} is the observed satellite TOA-BT. These double differences are calculated for each satellite channel.

The observed atmospheric correction will show some variability because of noise in the observations (drifting buoy SST and satellite radiances) and errors in the model results (NWP and CRTM forward modeling). Averaged over many cases, however, the differences should be zero if there are no biases. If biases are detected, and they are consistent across all three channels, then that would indicate a problem in the atmospheric prior information. Alternatively, if the biases differ among the channels then that would indicate a problem with the CRTM forward model. For the detection and correction of radiance operator biases we use the NAVOCEANO drifting buoy matchup data base (MDB). The MDB contains all of the variables needed to solve Eq. 2, including the satellite geometry. The drifting buoy, satellite radiance matchup criteria used by NAVOCEANO is 25 km and 3 hours. The MDB is available daily for all of the satellites processed by NAVOCEANO. A 15-day time window of NAVGEM and MDB inputs are used in the bias correction calculations.

Figure 3 shows there is a systematic bias of the observed atmospheric correction with NAVGEM TCWV priors for METOP-A and NOAA-19. Similar results are seen for the other satellites (not shown). The bias exceeds 1°K as TCWV > 50 kg·m^{-2}. As expected, the bias is negligible for the transparent 3.7 µm channel 3. We assume that bias in the NAVGEM TCWV can be removed by correcting the forward model simulated radiances. This approach avoids the need to correct the vertical distribution of atmospheric water vapor. Guided by the shape of the biases we fit a quadratic regression model using least squares. The regression model is formulated with no
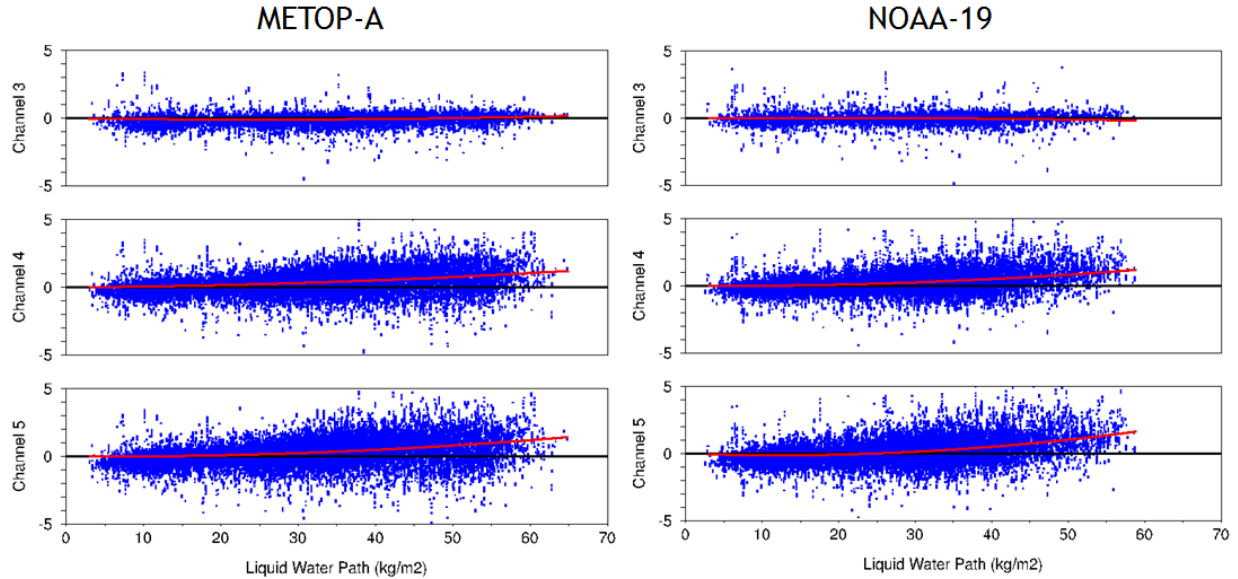
Figure 3. Dependency of prior (modelled) minus observed atmospheric correction to NAVOCEANO SST against NAVGEM total column water vapor. The dependencies are plotted for the 3.7 μm channel 3 (top), 11 μm channel 4 (middle), and 12 μm channel 5 (bottom), and METOP-A (left) and NOAA-19 (right) satellites. The least squares fit of these data to a quadratic function with zero intercept is plotted as a solid red line.

constant (intercept) term. This forces the bias correction model to be zero when the TCWV is zero. The regression models for each channel are shown in Figure 3 as solid curves. The bias correction slowly increases as TCWV increases in accordance with the zero intercept and quadratic formulation of the regression model. The model provides an adequate fit to the data over the range of observed TCWV. As will be shown, bias correction of the CRTM forward model radiances for the 11 μm and 12 μm channels results in zero bias in the SST corrections calculated from the SST inverse model.

Forward modeling of GOES-13 and GOES-15 radiances using CRTM, however, show a calibration problem with the GOES 3.7 μm channel 2 data. Figure 4 shows a nearly constant offset of the CRTM simulated radiances compared to the GOES-15 observed radiances for channel 2. This offset is not seen in the CRTM simulations of GOES-15 channel 4 data. This inconsistency across channels indicates a potential error in the CRTM forwarding modeling of GOES data. Alternatively, the offset could be indicative of an error in the calibration of GOES radiances by NAVOCEANO. The exact cause of the GOES channel 2 calibration errors is unknown. To correct for the offset we fit a linear regression model to the CRTM simulated
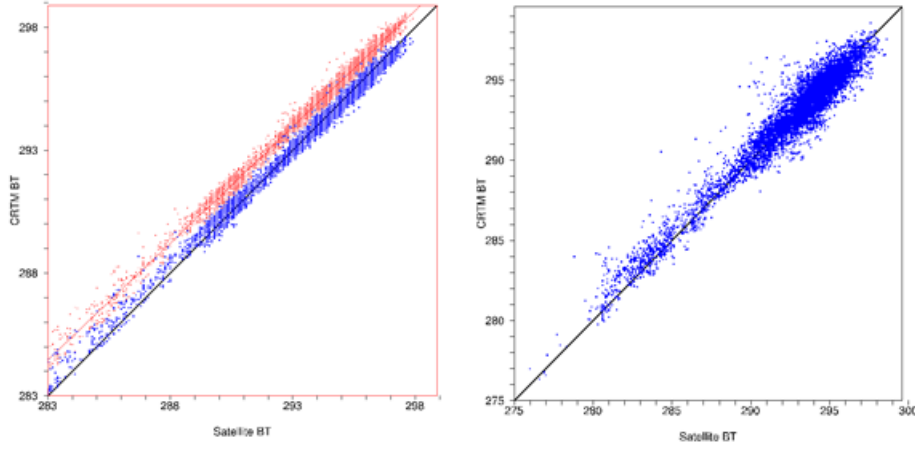
Figure 4. Scatter plots of observed (x-axis) versus radiative transfer model simulated (y-axis) brightness temperatures for GOES-15 3.7 μm channel (left) and 11 μm channel (right). The red dots in the 3.7 μm channel panel are observed GOES-15 brightness temperatures. The blue dots are brightness temperatures corrected by the linear calibration regression model indicated by the solid red line in the 3.7 μm panel.

radiances and remove the calibration error to obtain unbiased forward model results. This regression line is also plotted in Figure 4 along with the observed and calibrated radiances. The GOES-13 and GOES-15 channel 2 calibration models are calculated at the same time as the TCWV bias correction using the 15-day time window of MDB data. The GOES calibration coefficients are saved with the bias correction coefficients and applied in the observation operator. Bias correction coefficients valid 5 September 2013 are shown in Table 1. The

Satellite	Channel 3		Channel 4		Channel 5	
	x	x^2	x	x^2	x	x^2
GOES-13	-0.01312	0.00029	-0.05324	0.00115	-	-
GOES-15	-0.12113	0.00032	-0.04357	0.00101	-	-
METOP-A	-0.00958	0.00020	0.00008	0.00039	-0.00652	0.00056
METOP-B	0.00284	0.00009	0.00222	0.00023	-0.01895	0.00064
NOAA-18	-0.01557	0.00028	-0.01425	0.00067	-0.02331	0.00092
NOAA-19	-0.00125	0.00003	-0.00901	0.00063	-0.02357	0.00100
NPP-VIIRS	-0.00379	0.00018	-0.03842	0.00092	-0.03952	0.00103

Table 1. NAVGEM TCWV bias correction model coefficients for satellite channels. The coefficients are provided for the two terms of the quadratic regression model (x and x^2). Note that for GOES satellites channel 3 is actually channel 2 and channel 5 is not defined.

quadratic regression model coefficients are listed for each satellite and for each channel. The coefficients have been computed using 15 days of MDB data. Table 2 gives the calibration

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coefficients computed for GOES-13 and GOES-15 and Table 3 gives the combined radiometric noise and forward modeling errors for the different satellites and channels. All of these Tables are automatically updated when the bias correction software is executed. The coefficients are used every time the operator is executed in either of the applications described in section 4.

Satellite	Slope	Intercept	Mean Offset
GOES-13	0.931	21.073	-0.842
GOES-15	0.955	13.992	-1.000

**Table 2. GOES channel 2 calibration coefficients.**

Error Statistics. The SST inverse model requires specification of the prior errors. For the NWP priors we estimate uncertainty from the operational Navy Operational Global Atmospheric Prediction System (NOGAPS) ensemble.[1] The NOGAPS ensemble is executed on a T159 Gaussian grid (~1° resolution) using 80 members, with 20 members randomly selected for the error calculations. Each NOGAPS ensemble member initial conditions include perturbations to atmospheric wind, temperature, specific humidity, and terrain pressure. The perturbations to

Satellite	Channel 3	Channel 4	Channel 5
GOES-13	0.384	0.915	-
GOES-15	0.353	0.873	-
METOP-A	0.236	0.740	0.905
METOP-B	0.338	0.674	0.841
NOAA-18	0.230	0.713	0.903
NOAA-19	0.201	0.638	0.811
NPP-VIIRS	0.266	0.691	0.859

Table 3. Combined radiometric and forward model error standard deviations for the channel wavelengths on the satellites processed by NAVOCEANO. Note that channel 3 is actually channel 2 on GOES and that channel 5 is not available on GOES.

wind and temperature are calculated for all vertical levels of the numerical model, while the perturbations to specific humidity are calculated for those vertical levels between the surface and roughly 300 hPa. The perturbations to the NOGAPS analysis are generated in a single, unified process using a nine banded local formulation of the ensemble transform (ET) method (McClay

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[1] The global atmospheric ensemble will transition from NOGAPS to NAVGEM and increase in horizontal resolution (1 degree to 0.5 degree) and number of vertical levels (42 to 50) in early 2014. Beyond that a new version of the NAVGEM ensemble generation scheme is under development that will include a diurnal SST model and perturbations to both atmospheric variables and SST (McClay *et al.*, 2012).
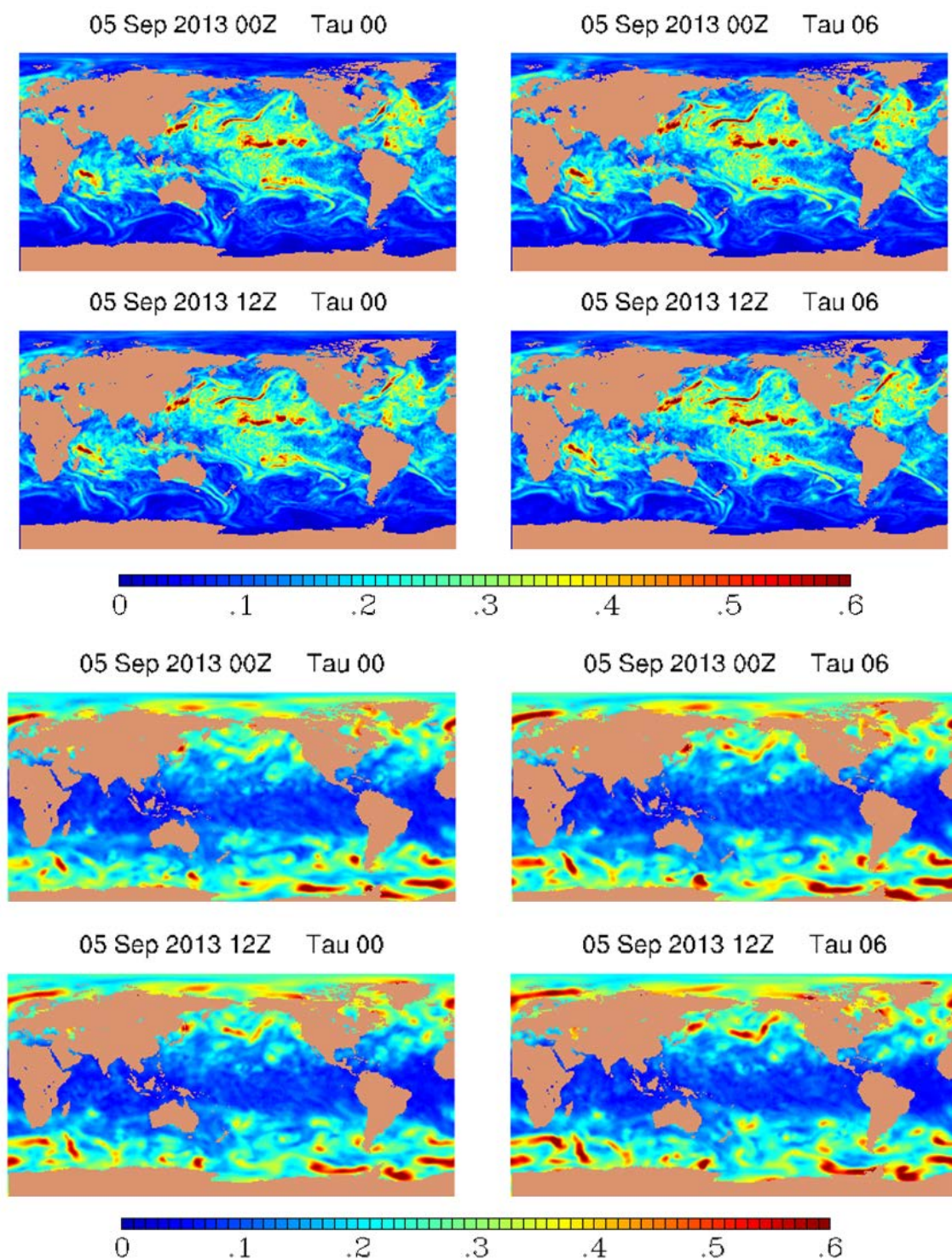
Figure 5. NOGAPS ensemble variability of specific humidity (top) and air temperature (bottom). The valid time and forecast period (tau) of the subpanels are indicated.

et al., 2010). The ET is executed twice a day on the 00Z and 12Z watches. Forecast fields from

the ensemble are available every 6 hours. The air temperature and specific humidity ensemble

member fields are vertically integrated since atmospheric variables are assumed to not vary with height in the SST inverse model. This is a good assumption for the SST window channels since the satellites observe surface emissions through the entire atmosphere. Figure 5 shows the variability of the integrated TCWV and air temperature fields on 5 September 2013. There are distinct differences in the variability patterns of the two variables. Air temperature variability is greater at high latitudes, while the maximum variability of TCWV is at low latitudes. Synoptic scale features (ITCZ, filaments along fronts between atmospheric pressure systems) are clearly seen in the variability maps.

The impact of these differential patterns of air temperature and TCWV variability are modulated in the SST inverse model by the magnitudes of the radiance sensitivity vectors contained in the Jacobians. Figure 6 shows representative examples of water vapor and air temperature Jacobians
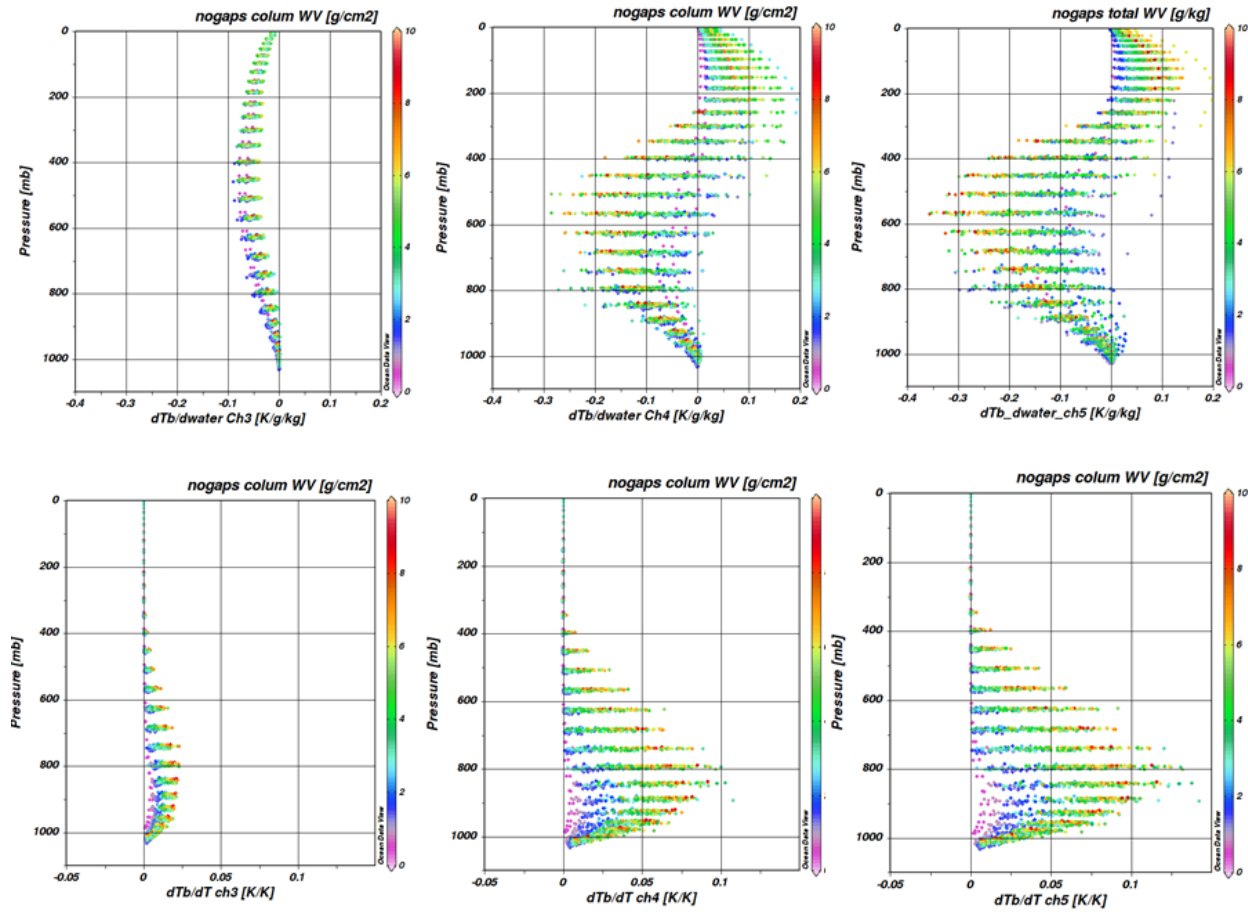
Figure 6. Jacobian vectors from CRTM using NOGAPS priors: (top) water vapor, (bottom) air temperature. The color coding of the Jacobian vectors reflect NOGAPS model water vapor concentrations.

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from CRTM for the 3.7 μm, 11 μm, and 12 μm channels on NOAA-19. The different Jacobian profiles represent different geographic locations in the global NWP model. The profiles are color coded based on the TCWV at the NWP profile location. The Jacobian for air temperature expresses the BT change at the TOA due to a 1°K change in atmospheric temperature at a given pressure level. Similarly, the Jacobian for water vapor represents the change in BT due to a unit change in water vapor concentration. The water vapor and air temperature Jacobians clearly have different vertical structures, but more importantly a change in TOA-BT is an order of magnitude more sensitive to changes in water vapor than air temperature.

In the ocean data assimilation application of the radiance operator, SST error is obtained from the NCODA 3DVAR temperature background errors. Background error in NCODA is computed from differences between successive forecasts at the update cycle interval. Since the forecasts are separated in time by an assimilation step the models are on different trajectories and include the influence of the observations. An inverse time weighted history of forecast differences is used to improve the estimate due to sampling limitations while at the same time allow the error fields to represent more recent events. The scheme is designed to provide background errors that: (1) are appropriate for the time interval at which data are inserted into the model; (2) are coherent with the variance of the innovation time series; and (3) reflect the variable skill of the model across the domain. Figure 7 shows SST background errors from the global HYCOM system valid 5 September 2013. SST is defined here as the top level of the model. SST
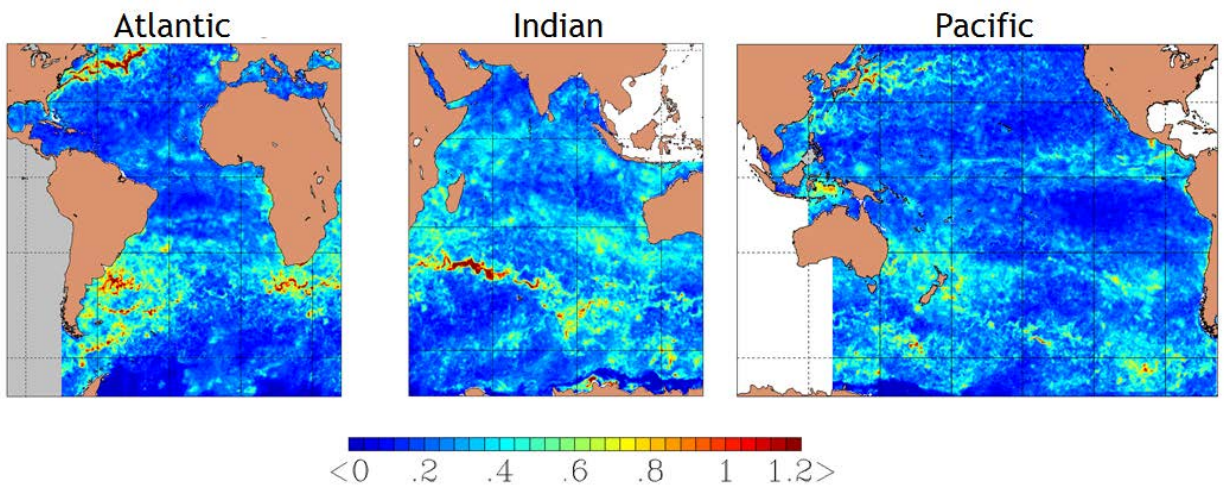
Figure 7. Top level of the model background temperature forecast error standard deviations in the global HYCOM/NCODA system.

variability is greatest in the tropics, Antarctic Circumpolar Current, and western boundary currents where oceanographic variability is high.

In the atmospheric correction application of the radiance operator, SST error is obtained from the error assigned to the retrieval by NAVOCEANO. These errors vary with satellite and retrieval type (day, night, relaxed day), but they do not vary with location. The errors are computed using a sliding time window of 30 days of differences between NAVOCEANO SST retrievals and collocated drifting buoy SST. Thus, the NAVOCEANO retrieval errors evolve with time and reflect changes in sensor calibration or sensor drift. Table 4 shows NAVOCEANO derived SST errors for different satellites and retrieval types valid 5 September 2013.

	N-18	N-19	MET-A	MET-B	G-13	G-15	VIIRS
Day	0.416	0.461	0.433	0.460	0.989	0.612	0.522
Night	0.440	0.411	0.395	0.382	0.587	0.544	0.405
Rlx Day	0.494	0.463	0.459	0.481	-	-	-

Table 4. Example of errors assigned by NAVOCEANO to empirical SST retrievals based on satellite and retrieval type (day, night, relaxed day). Satellite identifications in order from left to right are: NOAA-18, NOAA-19, METOP-A, METOP-B, GOES-13, GOES-15, NPP-VIIRS. Relaxed day retrieval type is not defined for GOES-13, GOES-15, and NPP-VIIRS.

Prior Corrections. Examples of prior corrections from the radiance assimilation operator executed in atmospheric correction mode are illustrated here using METOP-A global area coverage radiance data on 5 September 2013. A total of 511,179 METOP-A observations were processed. The NWP priors are 3-hourly forecasts from NAVGEM, and the SST prior is the NAVOCEANO empirical retrieval. The NAVGEM specific humidity priors have been bias corrected. Figure 8 shows the geographic distribution of the prior SST corrections. The corrections are plotted separately for day and night (ascending versus descending orbits). The major pattern in the SST corrections is a warming of the NAVOCEANO retrievals at high latitudes. This pattern is an illustration of a globally defined retrieval algorithm having a significant regional bias. As has been noted, there is considerable geographic and temporal variability in the atmospheric and oceanographic variables that control satellite TOA-BTs. The NAVOCEANO retrieval algorithm does not contain enough information to account for this variability other than the SST itself and an approximation of the atmospheric TCWV via the
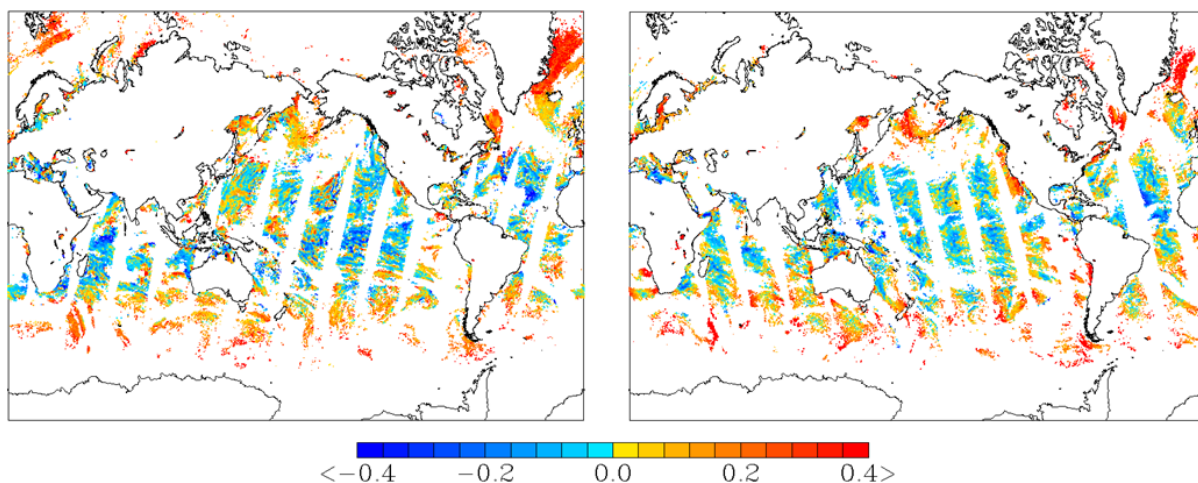
Figure 8. Geographic distribution of SST corrections for METOP-A on 5 Sep 2013. Day time observations are plotted on the left and nighttime observations are plotted on the right. The locations of the METOP-A radiance observations are color coded based on the magnitude of the SST correction from the inverse model. Warm colors indicate positive SST corrections; cool colors indicate negative SST corrections.

split-window algorithm. These limitations translate into regional biases in retrieved SST. There have been some attempts at deriving regional coefficients to reduce retrieval errors (e.g. Lat-Band Pathfinder, Casey *et al.*, 2010), where the variability of SST for a given region and season are embedded directly into the retrieval coefficients. Fundamentally, however, empirical SST retrievals cannot be improved without introducing additional information. Effectively, the radiance assimilation operator does that by using prior knowledge of the atmosphere at a particular time and place. The cold bias in the NAVOCEANO retrievals is due to the relatively dry atmosphere at high latitudes. A dry atmosphere is more transparent than a moist atmosphere. The NAVOCEANO retrievals are tuned to a moist atmosphere at lower latitudes where the drifting buoy matchups are more plentiful. As shown here, the geographic pattern of this cold bias error can be simulated effectively using radiative transfer modeling with NWP fields.

Figure 9 shows observation density plots of the SST inverse model correction versus liquid water path for METOP-A, METOP-B, NOAA-18, and NOAA-19 on 5 September 2013. The plots consistently show a greater number of positive SST corrections at TCWV < 20 kg·m^{-2} for all satellites. This result is not surprising since the same drifting buoy network is used by NAVOCEANO to derive retrieval coefficients for each satellite. METOP-B shows an interesting increase in the frequency of negative SST corrections for TCWV > 40 kg·m^{-2}. This
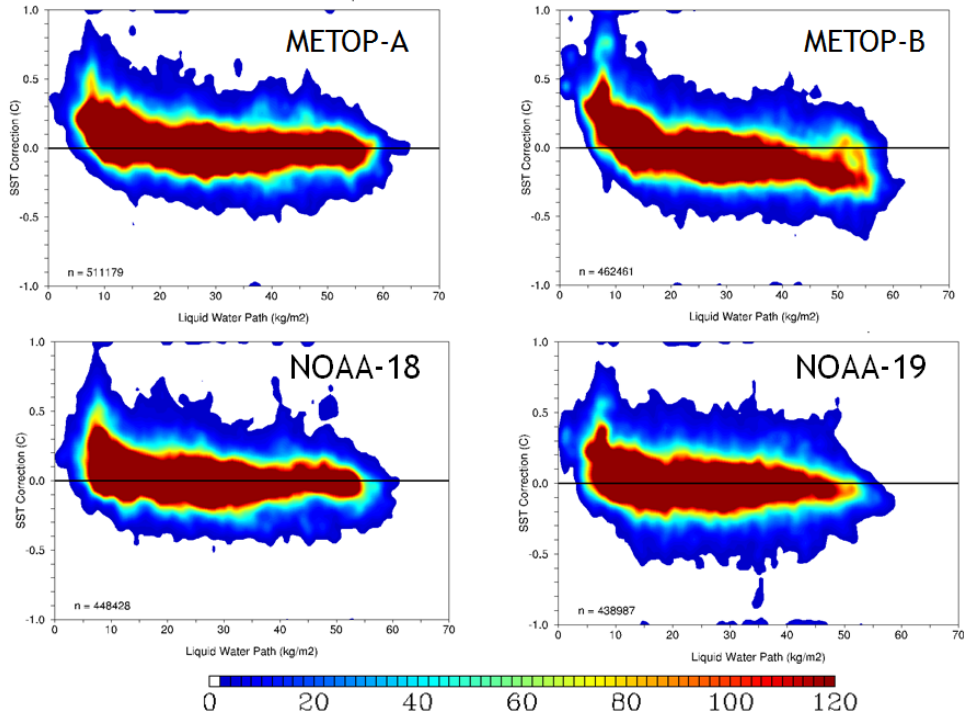
Figure 9. Observation density plots of METOP-A, METOP-B, NOAA-18, NOAA-19 SST corrections versus NAVGEM TCWV on 5 Sep 2013. Color sliced areas indicate observation densities of 2 or more observations. The number of observations plotted is indicated in the lower left corner of the subpanels.

pattern is consistently seen for METOP-B data every day. The exact cause of the pattern is unknown. No bias has been found in the forward modeling of METOP-B using CRTM and the METOP-B bias correction of the NAVGEM water vapor fields is very similar to that of METOP-A shown in Figure 3. Other than METOP-B, the observation density plots in Figure 8 show no bias in SST corrections at high TCWV. This confirms that the bias correction of the NAVGEM water vapor priors is working properly. Finally, the observation density plots show the occurrence of SST corrections on the order of ~1°K (colored blobs along the top and bottom of the satellite panels). These large corrections are clearly outliers and probably reflect erroneous radiance data. Thus, outcomes of the SST inverse model can be used as an additional quality control check on the NAVOCEANO TOA-BTs.

Geographic distributions of air temperature and TCWV corrections calculated by the SST inverse model are shown in Figure 10. In general, air temperature corrections are greatest at high latitudes where air temperature variability is high. A similar pattern is seen for TCWV where the corrections are large at low latitudes in the vicinity of increased uncertainty in NAVGEM water
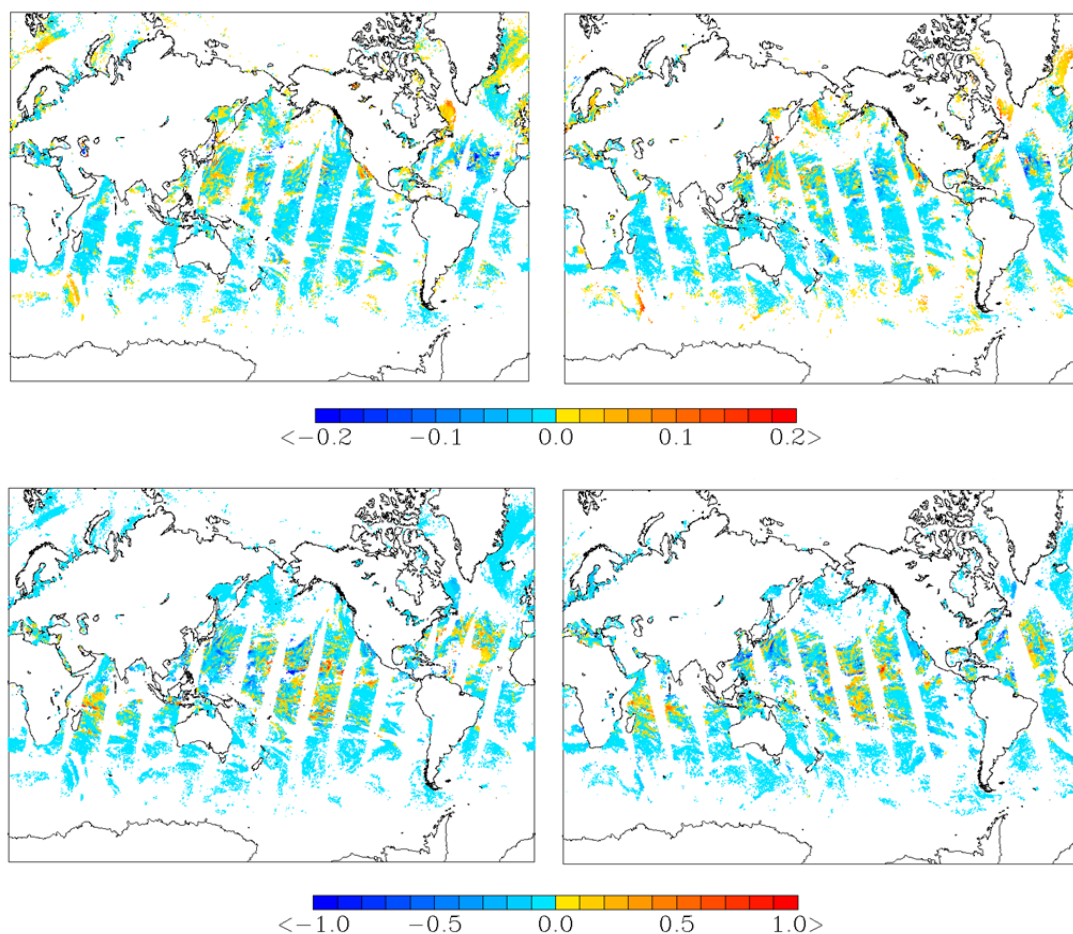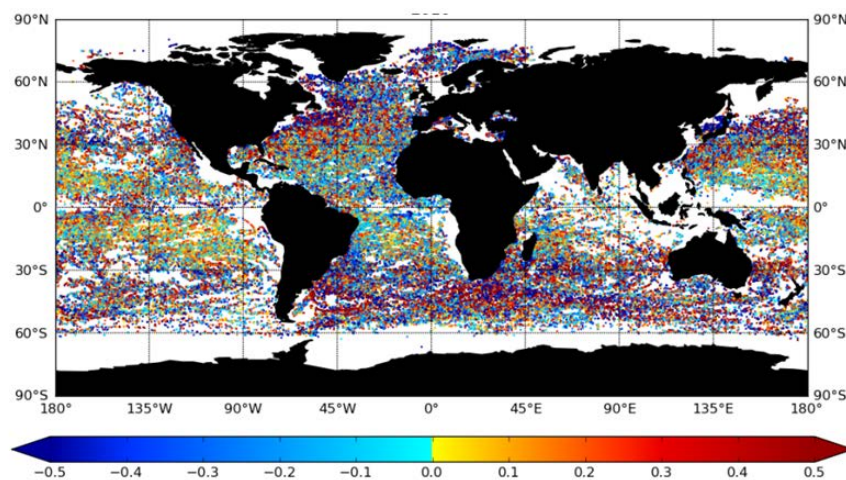
Figure 10. Geographic distribution of air temperature corrections (top) and TCWV corrections (bottom) calculated in the SST inverse model for METOP-A on 5 Sep 2013. Day time observations are plotted on the left and nighttime observations are plotted on the right. The locations of the METOP-A radiance observations are color coded based on the magnitude of the air temperature and TCWV corrections from the inverse model.

vapor content. These results illustrate the sensitivity of the SST inverse model to the specification of the error statistics. The δBT innovations are partitioned into corrections for air temperature, water vapor, or SST based on the relative magnitudes of the respective errors of the inverse model variables and the associated Jacobian sensitivity vectors. It is incorrect to assume that an observed change in TOA-BT for a satellite window channel is entirely due to a change in SST. The interleaving atmosphere between the ocean surface and the satellite must be taken into account.

Validation. Validation of the radiance assimilation operator was performed using a satellite SST data set obtained from the European Space Agency Climate Change Initiative (ESA-CCI). A

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description of the ESA-CCI is given in Hollmann *et al*. (2013). The ESA-CCI SST data set used here consisted of one year of METOP-A TOA-BTs for 2010. The radiances are collocated with the drifting buoy network and matched with air temperature and water vapor profiles from the European Center for Medium Range Weather Forecasting (ECMWF) model. SST from the Ocean Surface Temperature and Ice Analysis (OSTIA) system (Donlon *et al*., 2011) used as the temperature lower boundary condition by the ECMWF model is also provided. The ESA-CCI data set replicates the processing of NWP forecast fields and SST priors that support the radiance assimilation operator, including the collocation of drifting buoy SST ground truth observations. We compute SST corrections to the OSTIA prior SST using ECMWF model priors and CRTM forward and SST inverse modeling capabilities contained in the observation operator. We compare corrected SST to the collocated drifting buoy SST and determine if application of the radiance assimilation operator improves the fit of the prior SST to the buoy SST. Figure 11 shows the geographic distribution of the METOP-A cloud cleared radiances at the buoy locations for 2010. The color slicing indicates the error of the corrected prior SST relative to the in situ data. The mean error statistics are summarized in Table 5 by month and in Table 6 for the entire year. The SST radiance assimilation operator improves the prior SST for 10 months of the year.

Figure 11. Geographic distribution of drifting buoy locations matched to ECMWF and OSTIA SST fields in the ESA CCI data set for METOP-A in 2010. The locations of the buoy SST observations are color coded by the magnitude of the SST corrections from the SST inverse model.

The operator failed to improve the prior SST in 2 months of the year (April and September), but during those months the prior SST already was very close to the buoy SST (prior error < .01 °C). Averaged over the entire year at nearly 150,000 locations the radiance assimilation operator

showed an 80% improvement in the fit of the prior SST to the drifting buoy SST.

Month	Count	Prior Error	Corrected Error
Jan	12,074	-0.030	-0.004
Feb	11,577	-0.023	0.001
Mar	12,218	0.064	0.031
Apr	12,218	-0.003	0.021
May	13,354	-0.028	-0.002
Jun	12,269	-0.058	-0.032
Jul	14,016	-0.048	-0.024
Aug	13,401	-0.048	-0.025
Sep	13,237	-0.009	0.013
Oct	11,986	-0.021	0.004
Nov	11,547	-0.052	-0.025
Dec	11,941	-0.058	-0.031

Table 5. Mean error of prior and corrected SST versus drifting buoy SST for METOP-A TOA-BTs during 2010. The errors are listed by month along with METOP-A data counts. Prior error is the difference the OSTIA SST analysis and the drifting buoy SST. Corrected error is the differences the SST inverse model corrected OSTIA SST and the drifting buoy SST. Atmospheric prior information came from ECMWF model fields.

METOP-A Data Count	Error Prior SST	Error Corrected SST	Per Cent Improvement
149,383	-0.0314	-0.0062	80.2 %

Table 6. Summary statistics for SST inverse model corrections versus drifting buoy SST. See Table 5 legend for a description of the column headers.

6. Operational Implementation

The NCODA QC and NCODA 3DVAR systems are operational at the Navy centers: NAVOCEANO and FNMOC. Configuration of the NCODA system requires that the software and supporting data bases are identical at the two Navy centers. This section outlines the NCODA system changes needed to enable satellite SST radiance assimilation. For example, some of the information required by the assimilation operator is readily available at one center and not the other. Those differences are highlighted here. Basically, NOGAPS (NAVGEM) ensemble fields need to be made available at NAVOCEANO, and NAVOCEANO MDB files need to be made available at FNMOC.

SST radiance assimilation using NWP fields is more computationally costly compared to existing methods. First, there is the overhead of routine incorporation of NWP forecast and ensemble fields into the SST processing and the additional overhead of forward modeling of prior observations using the NWP fields. The new NCODA programs developed in support of the radiance assimilation operator have been parallelized using the Message Passing Interface (MPI). Parallelization is achieved by partitioning the incoming radiance observations among the processors. The problem scales well so it is anticipated that computational costs will not be a limiting factor provided there are enough processors to keep the number of observations allocated per processor at about $5 \cdot 10^4$. The high density, global 1-km radiance measurements from METOP-A, METOP-B, and NPP-VIIRS will necessarily require more processors than the lower density 4-km data. Implementation of the operator requires routine monitoring of differences between simulated and observed TOA-BTs, as well as monitoring of the quality of the SST corrections. The operator flow chart schematic shown in Figure 1 includes a *SST radiance monitoring* component. The graphics presented in this report have been generated by the system and can be used as a monitoring tool. However, other graphical and statistical outputs may need to be developed as we gain experience with the system. Nevertheless, the burden of additional monitoring of the radiance assimilation system outputs remains and needs to be addressed by the centers. Two new programs have been developed and NCODA 3DVAR has been modified to support direct assimilation of satellite SST radiances. The new programs are configured within the NCODA QC system and are briefly described here along with the changes made to the NCODA 3DVAR system.

NCODA_SST_BIAS. This program performs the NAVGEM water vapor bias correction and the GOES channel 2 calibrations. Inputs include a time history of NAVOCEANO MDB files and NAVGEM deterministic air temperature, specific humidity, and sea level pressure fields. Program control is achieved using command line arguments and environmental variables describing data directory paths. The environmental variables are the same as those currently used by NCODA QC. NAVGEM deterministic model fields are available at both NAVOCEANO and FNMOC. The NAVOCEANO MDB, however, is not available at FNMOC. The program uses a sliding time window of MDB and NAVGEM fields. The length of the time window is under user control, but tests have shown that a 15-day time window provides an

adequate number of matchups to ensure statistical reliability of the derived coefficients. The NCODA_SST_BIAS program is a stand-alone system and should be executed on a routine basis (daily or weekly) to capture drift in satellite calibrations or changes in NAVGEM model physics.

NCODA_SST.   This program performs the atmospheric correction application of the operator. Program control is achieved by command line arguments and environmental variables. The environmental variables are the same as those currently used by NCODA QC. NCODA_SST is executed prior to NCODA_QC and takes as input the satellite specific incoming files prepared by the NACOVEANO and FNMOC site specific QC data preparation programs. Different QC prep programs are used at the two centers since the decoding and data base storage of observations is completely different. The NCODA_QC incoming files already contain the observed TOA-BTs and associated satellite geometry information. NCODA_SST requires access to the NAVGEM deterministic and ensemble forecast fields. At the present time NAVGEM ensemble fields are not available at NAVOCEANO, although this may change in the future with the move of NAVGEM to increasing horizontal and vertical resolution and the development of a global coupled air/ocean forecasting system. These planned upgrades of the global system will require NAVGEM to be executed at the Navy DoD Supercomputing Resource Center (DSRC) in Mississippi, which is the operational computer system for NAVOCEANO. NCODA_SST command line arguments allow the program to process all satellites in sequence in a single execution or individually by separate executions of the program. The program appends the SST atmospheric correction to the NCODA_QC incoming file, where the follow-on execution of NCODA_QC saves the SST correction in the QC output files for use in the assimilation. The QC output files and assimilation file readers have already been configured to take the SST atmospheric corrections.

NCODA 3DVAR.   The NCODA data preparation step of the analysis has been modified to allow for assimilation of satellite SST radiances either directly or via the atmospheric correction calculated by the NCODA_SST program. For direct assimilation of satellite SST radiances a new ocean analysis namelist (*oanl*) variable has been defined: *sst_rad_asm*. If this namelist variable is set true the NCODA data prep program performs the CRTM forward and SST inverse modeling on the satellite TOA-BTs selected for the analysis space/time window and calculates

the corresponding SST correction. These SST corrections are added to the innovation vector file and assimilated simultaneously with all of the other data selected for the 3DVAR minimization. Alternatively, the pre-calculated SST corrections to the NAVOCEANO SST retrievals computed by the NCODA_SST program can be assimilated.   Here, *sst_rad_asm* would be set false and the ocean analysis namelist variable *phys_sst* would be set true.   The NCODA 3DVAR analysis will need access to NAVGEM deterministic and ensemble forecast fields for the direct assimilation of satellite SST radiances.

7.   Future Developments

The SST correction computed by the radiance assimilation operator will have multiple uses and benefits in Navy atmospheric and oceanographic forecasting systems. Use of a more physically based SST lower boundary condition in atmospheric data assimilation is expected to enable use of atmospheric sounder channels that have significant weighting near the ocean surface. Currently, observations from these channels are rejected in the atmospheric 4DVAR assimilation system because of the inaccuracies and temporal inconsistencies in the SST analysis dominated by the NAVOCEANO retrievals.   Inclusion of these near-surface sounder channels in the atmospheric model assimilation cycle will likely improve the NAVGEM model depiction of the marine boundary layer, which in turn will improve the derived fluxes used to force Navy ocean circulation models.

The radiance assimilation operator can be expanded to include the effects of aerosols; the presence of which tend to introduce a cold bias in infrared estimates of SST in important geographic locations, such as tropical cyclone genesis regions. The current limiting factor of dealing with aerosol contamination in TOA-BTs is accurate knowledge of the characteristics and amount of aerosol in the atmosphere at the time and location of the radiance measurement. Aerosol transport models can be used to provide this information. For this purpose, forecast profiles of aerosol optical depth from the Navy Aerosol Analysis Prediction System (NAAPS) can be integrated into the CRTM forward and SST inverse models. Eventually, NAAPS will be integrated into NAVGEM providing seamless predictions of the atmospheric state including atmospheric constituents. In addition, development of a NAAPS ensemble using forcing from the NAVGEM ensemble is underway. As stated in section 2, the radiance assimilation operator

is designed to incorporate all atmospheric variables known to affect SST. The inclusion of aerosols in the system is therefore a high priority. Finally, the radiance assimilation operator can be applied to ice covered seas to determine a correction to a prior ice surface temperature. Ice surface temperature is used in both Navy NWP and ice forecasting systems. Knowledge of ice surface temperature is important since it controls snow metamorphosis and melt, the rate of sea ice growth, and modification of air–sea heat exchange.

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